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The Cambridge Structural Database: a quarter of a million crystal structures and rising

FH Allen - Acta Crystallographica Section B Structural Science, 2002 - dx.doi.org
... Chemical **connection table** (see text and Fig. ... Formal two-dimensional chemical **structure
diagram** in terms of atom and bond ... Space group and **symmetry** operators. ...
Cited by 1140 - Web Search - journals.iucr.org - scripts.iucr.org - ncbi.nlm.nih.gov - all 6 versions »

SMILES. 2. Algorithm for generation of unique SMILES notation

D Weininger, A Weininger, JL Weininger - Journal of Chemical Information and Computer Sciences, 1989 -
pubs.acs.org
... beyond 15. Partial characterization is therefore often attempted and is adequate
for most **symmetry** perception problems. Such algorithms ...
Cited by 66 - Web Search - pubs.acs.org - csa.com

Computer storage and retrieval of generic chemical structures in patents, 2. GENSAL, a formal

...
JM Barnard, MF Lynch, SM Welford - Journal of Chemical Information and Computer Sciences, 1981 -
pubs.acs.org
... FORMAL DESCRIPTION OF GENSAL **Structure Diagram** Input ... a routine to convert its output
into the **connection table** ... that there are no **symmetry** considerations involved ...
Cited by 8 - Web Search

Chemical structure representation for information exchange Thomas Engel, Johann Gasteiger The ...

T Engel - Online Information Review, 2002 - emeraldinsight.com
... limitations of a **connection table** description: a ... Helson, HE (1999), "**Structure diagram**
generation", Reviews ... numbering and constitutional **symmetry**", Journal of ...
Cited by 1 - Web Search - emeraldinsight.com - ingentaconnect.com - ingentaconnect.com

Chemical Abstracts Service Chemical Registry System. 13. Enhanced handling of stereochemistry

JE Blackwood, PEB Jr., SW Layten, DH Lillie, AH ... - Journal of Chemical Information and Computer Sciences,
1991 - pubs.acs.org
... search or display of stereochemistry in the **structure diagram**. ... the octa- hedral center
in the **connection table** would be ... one or more of its **symmetry** axes leads ...
Cited by 1 - Web Search

Structural Search Codes for On-Line Compound Registration

LA Evans, MF Lynch, P Willett - Journal of Chemical Information and Computer Sciences, 1978 - pubs.acs.org
... rep- resentation, any unambiguous representation for a structure, eg, a **connection
table** derived from an arbitrarily numbered **structure diagram**, may be used to ...
Web Search

Simulation and Evaluation of Chemical Synthesis. Representation and Manipulation of S tereochemis ...

WT Wipke, TM Dyottlb - J. Amer. Chem. Soc, 1974 - pubs.acs.org
... trans- form a three-dimensional structure or a two-dimensional structural diagram
having wedged and hashed bonds into the ordered-list **connection table**, and to ...
Web Search

Computer Storage and Retrieval of Generic Chemical Structures in Patents, 16. The Refined Search: An ...

JD Holliday, MF Lynch - Journal of Chemical Information and Computer Sciences, 1995 - pubs.acs.org
... in which case they can be represented by a **structure diagram** or they ... are the full
computer representation (the extended **connection table** representation3 or ECTR ...
Cited by 3 - Web Search

CML tools and information flow in atomic scale simulations

J Wakelin, P Murray-Rust, S Tyrrell, Y Zhang, HS ... - Mol. Simul, 2005 - eminerals.esc.cam.ac.uk
... of molecular mass, chemical **structure diagram** generation, topologi ... 5. Apply **symmetry**
operations to generate the mini ... 6. Generate a **connection table** (CT) for the ...
Cited by 8 - View as HTML - Web Search

Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles

P Murray-Rust, HS Rzepa - Journal of Chemical Information and Computer Sciences, 1999 - www-encore.enscm.fr
Page 1. Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles
Peter Murray-Rust* ,† and Henry S. Rzepa ‡ Virtual School ...
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UP

CCL February 12, 1997 [004]

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From:	badertscher &at& org.chem.ethz.ch (Martin Badertscher)
Date:	Wed, 12 Feb 1997 17:30:55 +0100
Subject:	perception algorithms for aromaticity etc.

Software Archive
An archive of computation chemistry related software,

List Archive
An archive of all past messages on the ccl mailing list,

Data Archives
Collections of data sets of use to computational chemists,

Document Archives
Collections of faq's and other documentation for various different programs,

Search CCL
Text Search, RegExp Search,

Dimitris K. Agrafiotis wrote:

> We are trying to find some good algorithms for perceiving aromaticity,
> tautomerism and stereochemistry (RS, cis/trans) from a connection
> table, and algorithms for canonicalizing molecular graphs.

1. Canonicalizing molecular graphs
A molecular graph, or "constitution", can be coded as a connection table i more than one way. To prove that two connection tables code the same constitution is called the isomorphism problem. To solve the problem is notoriously expensive. One possible solution is to assign a canonical nam (or canonical connection table) to the constitutions. If two such names are the same, the constitutions are too. This involves the perception of topological symmetry. Many algorithms have been proposed, e.g., the far Morgan algorithm:

H. L. Morgan, J. Chem. Doc., Vol. 5 (1965) p. 107

Most of them, including the Morgan algorithm, suffer from the fact that they are not rigorous. Shelley has published an "almost rigorous" algorithm:

C. A. Shelley et al., J. Chem. Inf. Comput. Sci., Vol. 17, No. 2 (1977) p. 1

Ray Carhart, the wizzard, has found a counterexample (by summoning lo

R. E. Carhart, J. Chem. Inf. Comput. Sci., Vol. 18, No. 2 (1978) p. 108

As a reaction Shelley placed a brute force algorithm on top of his former one. The resulting construct is rigorous:

C. A. Shelley et al., J. Chem. Inf. Comput. Sci., Vol. 19, No. 4 (1979) p. 2.

Due to Carhart's punishment the authors were too careful in writing their text. So the scientific community missed the fact that the problem was solved for almost 10 years. Chemists normally don't read mathematical journals where such problems are addressed in much more cryptic ways.

I can dig out the FORTRAN77 code of the complete algorithm to canonic a connection table. It could certainly be translated easily into a more appropriate language. The copyright is with Morton E. Munk, Prof. of Chemistry at Arizona State University. He is surely willing to share the code with you. Contact me if you are interested.

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2. Perceiving stereochemistry
This is a much more complicated problem as it (sensibly) involves the stability of molecules, not only mathematics. To my knowledge there is or a single algorithm published and coded that generates all stable stereoisomers out of a canonical connection table. It has its origin in Munk's lab too:

M. Razinger et al., J. Chem. Inf. Comput. Sci., Vol. 33, No. 6 (1993) p. 81

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3. Perceiving aromaticity
Before the question of perceiving aromaticity can be addressed, it must b clear what the results are used for. You have to clearly define what aromaticity is. This can be done in a purely mathematical way. Benzene, furane, and thiophene might be considered aromatic in this way, butadier could be non-aromatic, cyclobutadiene and cyclooctatetraene anti-aroma If you consider chemical behaviour such as reactivity, benzene and thiophene could be considered aromatic. Furane, butadiene, and cyclooctatetraene are non-aromatic. Cyclobutadiene is anti-aromatic and therefore rather unstable.

Martin Badertscher, head of radiochemistry,
dpt. of organic chemistry, federal institute of technology, Zurich, Switzerla

E-Mail: badertscher[AT]org.chem.ethz.ch

Similar Messages

02/27/1995: Summary: Ring perception algorithms
03/11/1996: Law of conservation of difficulty: violations.
05/03/1995: summary (II): teaching material for computational chemistry
05/03/1995: undergrad computational chem
04/23/1992:   Huckel MO Theory software
10/01/1993: torsion of conjugated systems -- summary

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Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	2010	connection adj table	USPAT; EPO	OR	OFF	2006/01/19 20:48
L2	2	symmetry same 1	USPAT; EPO	OR	OFF	2006/01/19 20:48
L3	65	symmetry and 1	USPAT; EPO	OR	OFF	2006/01/19 20:49
L4	1614	structure adj diagram	USPAT; EPO	OR	OFF	2006/01/19 20:49
L5	2	3 and 4	USPAT; EPO	OR	OFF	2006/01/19 20:49

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CCL October 06, 1997 [009]

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List Archive
An archive of all past messages on the ccl mailing list,

Data Archives
Collections of data sets of use to computational chemists,

Document Archives
Collections of faq's and other documentation for various different programs,

Search CCL
Text Search, RegExp Search,

From:	Joerg Weiser <joerg { *at * } still3.chem.columbia.edu>
Date:	Mon, 06 Oct 1997 16:31:29 -0400
Subject:	Summary: Recognition of compounds from a connection table

Some time ago, I posted the following question:

"Do you know of any references that deal with the recognition of compounds (e.g stored in a compound library) from their connection tables?"

I received two answers. Thanks a lot.

===:

Try Ash, J., Chubb, P., Ward, S., Welford, S., Willet, P.,
Communiaction, Storage and Retrieval of Chemical Information,
Ellis Horwood Series Chemical Science, Ellis Horwood Limited,
Chichester, 1985.

It is not new, and some important modern developments are missing,
but is is still a good overview about the basic principles
and technology.

Dr. Wolf-D. Ihlenfeldt
Computer Chemistry Center, University of Erlangen-Nuernberg
Naegelsbachstrasse 25, D-91052 Erlangen (Germany)
Tel (+49)-(0)9131-85-6579 Fax (+49)-(0)9131-85-6566
===:
References:

Balaban, A.T.; Mekenyan, O.; Bonchev, D. : Unique Description of
Chemical Structures Based on Hierarchically Ordered Extended
Connectivities (HOC -Procedures). I. Algorithms for finding Graph
Orbits and Canonical Numbering of Atoms., II. Mathematical Proofs, J.

Comp. Chem. 1985, vol. 6, pp. 538-551.

Corneil D .G., Kirkpatrick D.G. : A Theoretical Analysis of various Heuristics for the Graph Isomorphism Problem. SIAM J. Comp., 1980, v. 9, No. 2, pp. 281-297.

Figueras J. : Automorphism and Equiavalence Classes. J. Chem. Inf. Cor Sci., 1992, v. 32, pp. 153-157.

Fortin S. : The Graph Isomorphism Problem. Technical Report No. TR 96-20, Dept. of Comp. Sci. University of Alberta, Edmonton, 1996. ftp://ftp.cs.ualberta.ca/pub/TechReports/1996/TR96-20/ (gzip)

Golender V.E., Drboglav V.V., Rosenblit A,B. Graph Potentials Method and it's Applications for Chemical Information Processing. J. Chem.Inf.Comp.Sci., 1981, v.21, No. 4, pp. 196-204.

Goodman S.E., Hedetniemi S.T., Introduction to the Design and Analysis of Algorithms McGraw-Hill, New York, 1977.

Harary F. Graph Theory, Addison Wesley, Reading, MA, 1969.

Hendrickson J.B., Toszko G., Unique Numbering and Cataloguing of Molecular Structures. J.Chem.Inf.Comp.Sci., 1983, v. 23, pp. 171-177.

Herndon W.C. Canonical labelling and System of Linear Notation for Chemical Graphs. in Chemical Applications of Topology and Graph Theory., ed. by R.B. King, Elsevier, Amsterdam, 1983, 231-242.

C. Jochum, J. Gasteiger, Canonical Numbering and Constitutional Symmetry. J. Chem.Inf.Comp.Sci., 1977, vol. 17, pp. 113-117.

Liu X., Balasubramanian K., Munk M.E. : Computational Techniques for Vertex Partitioning of Graphs, J.Chem.Inf.Comp.Sci., 1990, v. 30, pp. 263-269.

Liu X., Klein D. J., The graph isomorphism problem, J. Comp. Chem., 12 (1991) n. 10, 1243-1251.

McKay B. D., Nauty User's Guide (version 1.5), Technical Report No. TR-CS-90-03, Comp. Sci. Dept., Australian National University, Canberra,1990. http://cs.anu.edu.au/people/bdm/nauty

B. D. McKay, Practical graph isomorphism, Congressus Numerantium 30 !1981) 45-87.

Miller G. L., Graph Isomorphism, General Remarks, J. Comp. Syst.

Sci. 30 (1979) 128-142

Morgan H. L., The Generation of a unique machine description for chemical structures - a technique developed at Chemical Abstracts Service, J. Chem. Doc. 5 (1965), 107-113.

Randic M. : On Canonical Numbering of Atoms in a Molecule and Graph Isomorphism. J.Chem.Inf.Comp.Sci., 1977, v. 17, No. 3, pp. 171-180.

Razinger, M.; Balasubramanian, K.; Munk, M.E. Graph Automorphism Perception in Computer-Enhanced Structure Elucidation. J.Chem.Inf.Comp.Sci., 1993, vol. 33, pp. 197-201.

Read, R.C., Corneil D.G., The Graph Isomorphism Disease, J. Graph Theory 1 (1977) 339-352.

G. Rucker, C. Rucker, Computer perception of constitutional (topological) symmetry: TOPSYM, a fast algorithm for partitioning atoms and pairwise relations among atoms into equivalence classes. J.Chem. Inf. Comp. Sci., 30 (1990) 187-191.

G. Rucker, C. Rucker, On Using the Adjacency Matrix Power Method for Perception of Symmetry and for Isomorphism Testing of Highly Intricate Graphs. J.Chem. Inf. Comp. Sci., 31 (1991) 123-126.

Schubert W., Ugi I. : Constitutional Symmetry and Unique Description of Molecules. J. Am. Chem. Soc. 1978, v.100, No. 1, pp. 37-41.

Shelley, C.A.; Munk, M.E. An Approach to the Assignment of Canonical Connection Tables and Topological Symmetry Perception. J.Chem.Ihf.Comp.Sci., 1979, vol. 19, pp. 247-250.

I. V. Stankevich, E. G. Gal'pern, A. L. Chistyakov, I. I. Baskin, M. I. Skvortsova, N. S. Zefirov, O. B. Tomilin, Spectral Theory of Graphs in Chemistry. 1. Projection Operators and Canonical Numeration of Graph Vertices. J. Chem. Inf. Comp. Sci., 34 (1994) 1105-1108.

Stankevitch M.I., Tratch S.S., Zefirov N.S. : Combinatorial Models and Algorithms in Chemistry. Search for Isomorphisms and Automorphisms o' Molecular Graphs. J.Comp.Chem., 1988, v. 9, No. 4, pp. 303-314.

M. Uchino, Algorithms for Unique and Unambiguous Coding and Symmel Perception of Molecular Structure Diagram. I, II, III. J. Chem. Inf. Comp. Sci., 1980, 20, pp. 116-126.

Ullmann, J.R. : An Algorithm for Subgraph Isomorphism. J. ACM, 1976, vol. 23, No 1, pp. 31-42.

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Similar Messages
01/15/1993: Third International Conference on Chemical Structures
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06/01/1992: Computers and CHemistry Symposia, ACS Aug 24-28th
08/03/1995: ACS Chicago - CINF Abstracts   - 29 pages document -
02/24/1992: COMP Program for ACS MTG in San. Francisco
10/01/1998: Reminder - Fifth International Conference on Chemical Stru
01/05/1994: Summary of 1994 conferences list
01/18/1995:   COMP Program for the Anaheim ACS Meeting
02/12/1997: perception algorithms for aromaticity etc.
03/06/1995: EHMO and ASED on organometallics (summary)

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